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AUTOMATING THE ANALYTICAL LABORATORIES SECTION, LEWIS RESEARCH CENTER, NATIONAL AERONAUTICS AND SPACE ADMINISTRATION: A FEASIBILITY STUDY

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G. W. Barton

March 15, 1979

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FOREWORD

Lawrence Livermore Laboratory performed this work for the National Aeronautics and Space Administration under task order number YCG6747.

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AUTOMATING THE ANALYTICAL LABORATORIES SECTION, LEWIS RESEARCH CENTER, NATIONAL AERONAUTICS AND SPACE ADMINISTRATION: A FEASIBILITY STUDY

ABSTRACT

We studied the feasibility of computerized automation of the Analytical Laboratories Section at NASA's Lewis Research Center. Since that laboratory's duties are not routine, we set our automation goals with that in mind. We selected four instruments as the most likely automation candidates: an atomic absorption spectrophotometer, an emission spectrometer, an x-ray fluorescence spectrometer, and an x-ray diffraction unit.

Our study describes two options for computer automation: a time-shared central computer and a system with microcomputers for each instrument connected to a central computer. A third option, presented for future planning, expands the microcomputer version. We determine costs and benefits for each option. And we conclude that the microcomputer version best fits the goals and duties of the laboratory and that such an automated system is needed to meet the laboratory's future requirements.

1. INTRODUCTION

OBJECTIVES

This study seeks to define current and future automation requirements of the Analytical Laboratories Section (ALS), Materials Characterization and Operations Branch, NASA Lewis Research Center (LeRC), Cleveland, Ohio. We propose several different alternative plans for fulfilling those requirements and present analyses of the costs and benefits of these alternatives. The basic data and information for this study was developed through interviews with the ALS staff.

ALS has already expended considerable effort attempting to automate some of its instruments. These efforts have resulted in some benefits, but have not been done under an overall integrated approach to laboratory automation that could easily be expanded or changed as the situation required. ALS has also benefited by using the central computer facilities at LeRC. We find, however, many disadvantages to an uncoordinated automation effort and in too heavy a reliance on remote computer facilities designed for sophisticated data reduction. We propose alternatives to overcome these disadvantages and hence to approach more closely the

ideal concept of laboratories that can perform many parameter determinations simultaneously, quickly, and accurately.

AUTOMATION EXPERIENCE AT LAWRENCE LIVERMORE LABORATORY

Since 1966, with the installation of the PDP-7 computer in its General Chemistry Division (GCD), Lawrence Livermore Laboratory (LLL) has been deeply involved with and in the forefront of computer automation of chemical analyses, both in time-shared and stand-alone modes. Since 1973, the Environmental Research Center of the U.S. Environmental Protection Agency (EPA) in Cincinnati and members of GCD, working together, have specified, designed, and placed in operation three laboratory automation systems. GCD has remained as a consultant to the EPA for continuing advice and service and to help develop new systems at other EPA laboratories. In addition, GCD has specified and installed automation systems for The U.S. Geological Survey (USGS) National Water Quality Laboratories in Denver and Atlanta.

ORGANIZATION OF STUDY

Section 2 of this report describes the ALS facilities and gives a general outline of the character of its laboratory. From this description we develop

goals and candidates for instrumentation in Section 3. In Section 4 we discuss several plans for automation. Section 5 discusses the components of these systems and summarizes the costs and benefits from details found in Appendices A, B, and C.

2. ANALYTICAL LABORATORIES SECTION

GENERAL DESCRIPTION OF LABORATORY AND FACILITIES

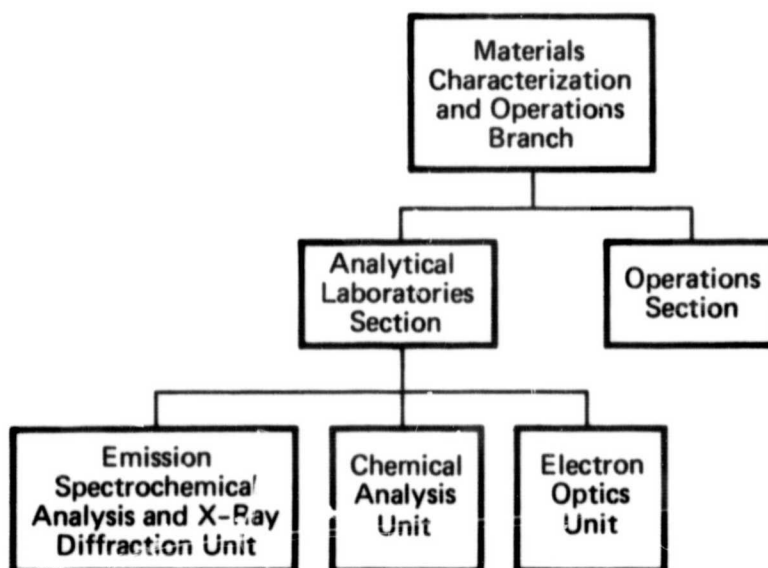
ALS is part of the Materials Characterization and Operations Branch, with William Gordon as its section chief. The section consists of 13 people, professional and technical. It has three units: the Emission Spectrochemical Analysis and X-Ray Diffraction Unit, the Chemical Analysis Unit, and the Electron Optics Unit (Fig. 1).

The Emission Spectrochemical Analysis and X-Ray Diffraction Unit has two emission spectrometers operating simultaneously from a common source, two x-ray diffractometers, and four x-ray sources for Debye-Scherrer and Guinier-de Wolff cameras. The Chemical Analysis Unit possesses one atomic-absorption instrument, an x-ray fluorescence unit, and three LECO instruments for inert-gas fusion, carbon determinations, and nitrogen-oxygen (N-O) determinations. It also has a vacuum fusion analyzer and the usual instruments associated with wet chemical analysis

such as analytical balances, pH meters, and two spectrophotometers. The Electron Optics Unit has a scanning electron microscope (available for use by outside operators), a scanning transmission electron microscope, and an electron microprobe.

The Central Computer Facility at LeRC consists of an IBM 360/67 computer operating in the time-share mode. Input to it comes mainly from a MODCOMP-III computer operating a 3-megabyte fixed-head disk called a "data collector". About a dozen PDP-11's located in a room adjacent to the 360 send data to the data collector. These PDP-11's are controllers and data concentrators for remote microcomputer-based data takers. Data may also be sent by terminal. This scheme works best for large data-generating experiments such as wind tunnel tests, but has not worked as well for chemistry instrumentation. Experiments depend on equipment availability and must be scheduled at least two days in advance. Uncertain response times are often not suitable for instruments that generate many small sets of data each day.

FIG. 1. The Analytical Laboratories Section (ALS) at Lewis Research Center, Cleveland, Ohio.



MISSION

The general ALS mission is to aid various LeRC facilities and contractors in their projects. The program in Cleveland now includes such projects as highway vehicle propulsion under primarily a Department of Energy transfer of funds, new types of wind turbines, and application of photovoltaic devices. Thus, much of the work consists of special problems and often requires a good deal of method development. In this respect, ALS's work is very similar to GCD's work at LLL. The samples are often unusual alloys, cermets, and specimens for troubleshooting problems with mechanical assemblies.

Analytical requests are for a wide range of measurements on a wide variety of materials. Some typical examples are identification of deposits left on a substrate, quantitative analysis of the components of an alloy, analysis of diesel exhaust, and determination of impurities in shale-oil fuel and how these impurities might affect corrosion problems. The laboratory participates in "round-robin" evaluations of analytical procedures, and it may be called to be the final judge in the arbitration of differences in analytical measurements. It also consults and advises on technical problems and recommends commercial analytical laboratories.

There are, however, a certain number of routine analyses. These analyses associated with specific projects may continue for the duration of the project. Hence, the overall work of the laboratory is an ever-changing mix of method development, sample running, and special problems.

HOW ALS FULFILLS ITS MISSION

It follows that ALS must use a variety of techniques in solving problems presented to it. That is, it must frequently develop new methods or modify existing methods. This varying sample type requires that ALS maintain personnel, expertise, and equipment able to respond quickly and competently.

As a result, ALS personnel have employed a number of techniques using computers to assist in gathering and interpreting data. Some of these computers are built into the instrument to control instrument settings, such as found in the x-ray fluorescence instrument; others are on direct line to

the central computer facility, such as with the emission spectrometer. For solving special problems in emission spectrometry and x-ray diffraction, ALS uses photographic plate readers. Sometimes data reduction is accomplished by entering data by hand either into a programmable calculator or into the central computer facility.

These computerization techniques have been successful enough to justify a more integrated approach to the automation of ALS facilities.

GENERAL SURVEY OF INSTRUMENTS

Chemical Analysis Unit

Besides doing conventional wet chemical analyses this unit works with three LECO instruments for determining carbon, oxygen, and nitrogen; an atomic-absorption instrument for trace metal analysis; and a vacuum fusion apparatus.

Atomic-Absorption Spectrophotometer (AAS), Instrumentation Lab Model-153. This AAS is around 10 years old. It is a double-channel instrument with two beams in each channel. Since we have automated an AAS like this before, it would be relatively inexpensive to transfer the automation to this one. This instrument is likely to be replaced soon and if so, a basic unit will be purchased. An AAS automated into a general system will give much more flexibility in operation than the currently available AAS's with built-in microprocessors. Such spectrophotometers are strictly limited to the software the manufacturer provides, and this software is generally directed toward multiple running of routine samples.

This concept is further supported if an inductively coupled plasma spectrometer (ICP) is purchased. The AAS will then be relegated to running samples, which the ICP is not as capable of doing, and flexibility of operation will be even more important.

We recommend that an AAS be automated and that it be one without an original-equipment microprocessor.

Inert-Gas Analyzer, LECO 734-100. This instrument is 15 years old, but is still used frequently for oxygen determinations in the range of 0.5 to 5% and for samples that do not release their oxygen fast enough for the LECO TC-30 instrument (see below). It uses an induction furnace to heat the

sample and convert the oxygen to carbon dioxide (CO_2). The CO_2 is eventually released from a molecular sieve trap, and the readout is from a thermal-conductivity cell. A Varian 475 digital integrator integrates the peak. The system is calibrated by injecting CO_2 through a gas-sampling valve and constructing a calibration curve.

Since this instrument uses a constructed calibration curve, it would be helped by online data taking, which could construct a calibration curve and return answers immediately. However, the instrument is 15 years old and is used only in special situations, so automation would have low priority.

N-O Determinator, LECO TC-30. This apparatus consists of a high-current furnace to combust the sample, a cupric oxide (CuO) furnace to convert carbon monoxide (CO) to CO_2 and a silica gel column to separate the CO_2 from the nitrogen (N_2). A thermal conductivity readout produces the signal which is read on two digital voltmeters; one for CO_2 and one for N_2 . A one-point calibration curve is used, and weight differences between standard and sample are compensated by means of a dial on the instrument. This instrument would benefit from automation designed to transfer the analytical results to a data management system for quality assurance calculations. Otherwise, automation would probably not improve the normal operation of the instrument.

Carbon Determinator, LECO ELC-12. This is the standard induction-furnace carbon determination in which the sample is burned in a stream of oxygen. The output comes from a thermal-conductivity cell. A LECO EB-26 electronic balance is wired into the apparatus, and this automatically inputs the weight of the sample. Readout is automatically in concentration. There is also a calibration control for weight corrections. This instrument also has a low priority for automation. A data management system might justify placing this instrument online.

Vacuum Fusion-Gas Analyzer, National Research NRC-912. This commercial vacuum fusion analyzer uses fusion in a platinum bath to release CO , hydrogen (H_2) and N_2 from samples. The combined total is measured by pressure-volume-temperature techniques (using a McLeod gage). The gases are then pumped over CuO and dried with magnesium perchlorate; then CO_2 plus N_2 is measured. Finally, the CO_2 is frozen out and N_2 alone is measured. This instrument is used

mostly for referee samples and to settle disputes. LLL's vacuum fusion analyzer now automated on our PDP-7 is generally similar in operation. A study of the problem of redesigning the software and hardware of LLL's vacuum fusion apparatus to move the system from GCD's PDP-7 to the modern ECLIPSE computer concluded that it would not be cost beneficial. In the LLL study the two most persuasive elements leading to this conclusion were that (1) the demand for vacuum fusion analyses was low and (2) when needed could be provided competently by commercial laboratories. Since the use factor for the ALS instrument is also low, the LLL conclusions probably apply to the NRC-912 vacuum fusion instrument. Thus it should not be automated.

X-Ray Fluorescence Spectrometer, Diano XRD-8000. This is a standard x-ray fluorescence setup with the Diano XRD-8000 controller and readout. It is used for both qualitative and quantitative analysis. Samples are often put into solution for analysis on the instrument. The XRD-8000 has a microprocessor that can control and display the settings of a number of parameters involving the x-ray generator, counting tube, pulse-height selection, amplifier gain, and scaler timer. The final readings are in counts and are printed on a teletype. Matrix corrections are not used as yet. A calibration curve is produced using an electronic calculator. Programs that handle the calibration and display the curves would be desirable. Also, the goniometer could be controlled by the computer for scanning. The control of the goniometer and calculational algorithms, using a long form and a short form of a modified Birk's matrix correction program, are currently being developed at LLL for another project. **LLL's expertise can be transferred to this instrument, which is a good candidate for automation.**

Emission Spectroscopy and X-Ray Diffraction Unit

Atomic Emission Spectroscopy. The laboratory has two emission spectroscopes: a 3.4-m Jarrell-Ash spectrograph and a 1.5-m Jarrell-Ash spectrometer. These instruments are optically coupled for simultaneous use with either a spark source or a controlled-atmosphere arc source. Data from the spectrometer are automatically sent to the computer center and filed on the disks of the 360/67. Data from the spectrograph will soon be read by a Joyce-Loebl reader, locally controlled by a PDP-11/05.

A fairly large effort has been expended to automate the 1.5-m spectrometer. At the present time this automation suffers from several faults ranging from noise problems to slow turnaround time. **LLL has automated an emission spectrometer and could apply this knowledge here.**

LLL has also automated a Jarrell-Ash microphotometer using a precision screw driven by a stepping motor. However, the screw drive would sometimes permit a line to be totally missed on automated plate scans. An interactive program, which allowed the operator to manually position the microphotometer head at the beginning of each line of interest and the computer to then take over the scan, was quite satisfactory for the quantitative analysis of selected elements.

The reading of the spectrographic plates would benefit from LLL experience with computer-assisted plate readers.

X-Ray Diffraction. This facility has two diffractometers as well as a number of Debye-Scherrer and Guinier-de Wolf cameras. These are used primarily for phase identification in metal and ceramic samples. An automated plate reader is available, but a satisfactory data reduction algorithm for the central computer facility has not been written. Automated readout, even if slow, would relieve the load on the staff. A faster way than the handsorting of recipe cards to access the standard crystallographic library would also be very desirable.

Much of the work in automating x-ray diffraction is now being done at LLL in another division. Whether a significant part of this work could be transferred to the NASA facilities depends on (1) the similarity between the work and (2) the degree of generality built into the LLL programs. The automated plate-reader data reduction algorithms would probably have to be developed as a separate project. **If this technology were transferred to ALS it would simplify automating at least part of the x-ray diffraction instrumentation.**

Electron Microscopy Unit

The Electron Microscopy Unit has two automated electron microscopes: one scanning, with a NOVA-1210 controller, and one transmission, with

a PDP-11/05. In addition to the usual studies, it would be desirable to find a way to reduce electron diffraction patterns produced in the transmission microscope. The unit also has an ARL electron microprobe. It outputs its data to a silent-700 teleprinter, but for final reduction the data is hand typed into the IBM 360.

The automation problems here are somewhat similar to the x-ray diffraction problems. In addition, the transmission microscope produces photographic plates, and it would be very desirable to have at least a computer-assisted readout for these. **The electron microprobe needs to be put online. The scanning and transmission electron microscopes need their outputs tied to a data management system.**

SAMPLE LOGGING, DATA FLOW, REPORTS, AND RECORD-KEEPING

About 95% of the samples received at ALS are walk-in samples. The remaining 5% are associated with continuing projects of some kind.

The person requesting analysis fills out a request form, submits the samples, and enters the appropriate data in a logbook. Each section keeps a separate logbook. Sample numbers are assigned consecutively as samples are received. Identifying numbers furnished by the requesters are also recorded. Local samples are shared with the other units. Reports are informal and varied depending on the information requested by the submitter. Often the requester discusses the problem directly with the analytical section involved.

The general atmosphere of the laboratory is informal and flexible, which is appropriate for handling a variety of analytical problems that often require discussion and method-development. Any automation system must take this situation into account and allow a maximum of interaction with the users. The automation system must also be versatile and allow for frequent user program changes while the user system is running and performing analytical determinations. **The large and varied number of requestors also suggests a data management system carefully designed to provide the proper inputs with a minimum of operator interaction.**

3. APPROACHES TO AUTOMATION

SCOPE AND RESTRAINTS

In our introduction we mentioned that ALS is a section of the Materials Characterization and Operations Branch. We recognize that other branches of the Materials and Structure Division would benefit from an in-house computer system. This study considers only a computer system that would address the needs of chemistry and closely related operations and allow ALS to handle a greater laboratory workload with quick response and high reliability.

Although LLL has been actively engaged in analytical chemistry computer automation for over ten years, and in transferring that expertise since 1973, some of the instruments covered in this study have not been included in any of the former projects. Thus, it is prudent that automation proceed in an orderly fashion.

GOALS OF ALS AUTOMATION EFFORT

The goals of ALS can be reduced to two fundamental objectives: (1) respond quickly to analysis requests and (2) perform analyses with optimum accuracy and reliability. These are continuing goals, and to meet them in the past has required acquisition of new analytical instruments and staff involvement in developing manual calculational and graphical methods. Further improvements are possible through the use of computer automation in the laboratory. The objectives are to provide the means to

- improve method development using a flexible system;
- link individual laboratory instruments into a system that will acquire and process data and perform quality control tests;
- store the data for subsequent recall for compilation of a summary analysis report;
- determine quality control results during the time samples are being run;
- assure the integrity of the analytical data and its retention (backup) so no data can be altered or lost;

- lessen the number of transcriptions of data and perform calculations more rapidly;
- reduce or eliminate possible errors made in the above steps;
- enter data offline from low-use and non-automated methods;
- log in samples, their identity, descriptions, the analyses requested, changes in analytical requests, and other information pertinent to the analyses to be performed and the eventual report to be compiled;
- determine the status of individual or groups of samples and the parameters completed relative to the study plan; and
- list work schedules of samples or parameters to be run.

CANDIDATES FOR INSTRUMENT AUTOMATION

Two of the instruments in the list have already been automated by LLL in previous projects. These are the atomic-absorption spectrophotometer and the direct-reading emission spectrometer (quantometer). LLL has software and hardware designs that would allow an economical implementation. At the present time another division of LLL is engaged in automating x-ray diffraction and fluorescence units used in metallographic applications. Many of the techniques developed in this automation project could be applied to ALS.

We have selected four instruments from those surveyed as the first candidates for computer automation. The emphasis on these four instruments does not mean that the other instruments have been ignored, but that current requirements will be better served by first developing a basic automation system with some representative instruments. This will enable ALS to evaluate the system and plan for optimization and expansion. Since photographic plates are a result of the x-ray diffraction unit and emission spectrograph as well as of other instruments, a system will be proposed that will be versatile enough to allow the future development of a plate reader and of a method to use data from existing plate readers.

We propose as an initial phase the automation of the AA spectrophotometer, the Diano XRF spectrometer, the emission spectroscopy direct reader, and an x-ray diffraction unit.

We also have included in the study a system encompassing all the instruments deemed suitable for automation. This system has been developed to show where an orderly approach might lead and to suggest ultimate costs.

4. ALTERNATIVE SYSTEMS FOR ALS AUTOMATION

FEATURES REQUIRED TO MEET AUTOMATION OBJECTIVES

This section describes the features required to achieve the automation objectives listed in Sec. 3.

- To maximize instrument capacity, the computer must be able to take readings from the instrument output at the time a sample signal is present and to sense and control the introduction of new samples. Concentrations are calculated immediately, and quality control checks are made onstream. On fully automatic instruments, the operator is notified immediately if something goes wrong with a run so it can be corrected. On semi-manual operations, the computer saves time between samples by relieving the operator of the need to read and calculate concentrations.

- Digital reading of the instruments by a computer is more objective than visual reading and often covers a broader dynamic range. In addition, accuracy is improved by using some of the increased sample capacity that the computer provides to run more standards, spikes, and duplicates.

- Computer automation provides two important kinds of quality assurance (QA). The first kind of QA is passive; it results from the fact that the flow of information is always under computer supervision, with no hand transcription of data once it is entered into the system. If the system makes a mistake, it is almost invariably the kind of mistake that humans find preposterous. Such errors are easy to spot.

- The second kind of QA provided by computer is active. The arithmetic power of the computer permits easy implementation of analysis algorithms and statistical tests, which are laborious to do by pencil and paper or even with a modern hand calculator. The analyst must prepare duplicate samples and standards and spike a certain fraction of samples. This added effort is minimal.

These two kinds of QA alert the operator to trends in system behavior and permit corrective action before, or as soon as, obvious false results are produced.

- The computer easily handles the tedious, repetitive work that operators have done in the past and frees them for tasks that better use their talents. There are several major ways the computer helps the analyst. It reads all the data and calculates the concentration of samples and the curves for standards, displaying this information immediately so the analyst can plan his work more effectively. With more extensive data storage, the analyst will be able to list a set of samples for a particular test from the system storage and to arrange the list of samples in a pattern that may include check standards and rerun samples. The analyst will be able to obtain a summary of work that needs to be done and work that has been done, and to create tables of output data. It will also be possible to retrieve stored data, interparameter quality control values, and acceptance limits to help with dilutions and alert operators and users to samples that need special attention.

- The computer saves clerical time and reduces clerical errors because it eliminates all hand transcription of information and data after the initial sample-identifying information has been entered. It will print reports suitable for filing or distribution and will maintain an inventory logbook.

- At least one month's accumulation of analysis data should be able to be stored in computer system files. These data can be associated with everything known about the sample. With the proper software, information can be made available in a variety of formats for report preparation. It can also be used to look at trends of instrumental behavior (for example, calibration drift), check quality control parameters, and prepare work accountability reports. Information on certain unique

analyses should be accessible through the computer indefinitely.

- An automation system should have certain other features to be effective. The computer system should easily be able to accommodate added instruments and perform added automatic functions. The need for help from personnel outside the automated laboratory should be minimized. The operator should be able to use the computer as a powerful calculator offline. The laboratory scientist must be able to make necessary changes when new information, procedures, and operations are instituted.

ALTERNATIVE SYSTEMS

We chose the alternative systems for ALS bearing in mind the scope, objectives, and restraints discussed earlier.

Alternative 1 and 1A. The candidate instruments and auxiliary services are tied to a central ALS host computer.

Alternative 2. Each candidate instrument is tied to its own microcomputer. These microcomputers are in turn connected to a central microcomputer along with the auxiliary services (point-to-point network).

Alternative 2A. The candidate instruments and auxiliary services are tied to an interconnected network of microcomputers (multinodal network).

Alternative 3. A combination of alternatives 1 and 2, which could handle all current instruments, allow for future expansion, and have complete data management facilities.

Each of the above systems would have a means of transmitting data to the Central Computer Facility of LeRC's Computer Services Division.

System 1

Figure 2 shows System 1. This system incorporates a minicomputer for time-shared data acquisition, processing, and control and for data management functions.

High-use analytical instruments are placed online to the time-share computer. Input/output terminals are available to each instrument, and data storage backup is provided by a magnetic tape unit at the computer.

The system should include appropriate input/output terminals at the online and offline instruments and the ability to program in high-level language.

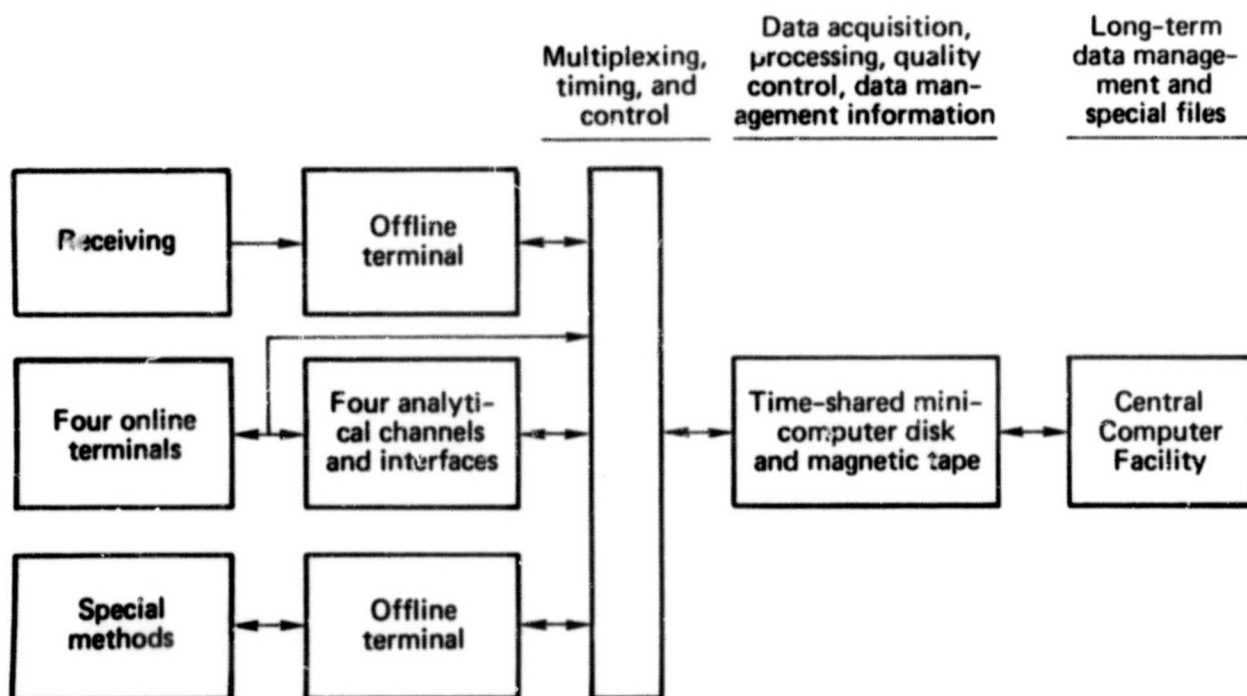


FIG. 2. System 1, which incorporates a time-shared minicomputer.

System 1A, A Variation of System 1

In-house data management is excluded from the system in favor of data management at LeRC's Central Computer Facility. A time-share computer would be used only for data acquisition, processing, and control for the high-use instruments.

Advantages of System 1

- The system can be added to in steps.
- A minimum version of the system can service all of the high-use instrumental methods on a time-share basis.
- The system is similar to other systems developed for the EPA's and USGS's water analysis laboratories. Therefore, certain hardware and software developments are transferable, with some savings in cost.

Disadvantages of System 1

- There is no backup for system downtime. When the system is being altered or repaired, in-

struments must wait. System programming must be scheduled carefully.

- The question of response time for the individual user becomes critical as more and more instruments are added to the system and if extensive data management is on the system.

- Although the orderly approach is possible from the instrument point of view, a large ALS host computer complicates orderly automation because the computer itself is such a large part of the overall system.

System 2

Figure 3 shows System 2, in which the fundamental building block is the microcomputer with a mass-memory device. The system comprises multiple units of the fundamental building block for online acquisition and processing of data from individual analytical instruments. The system also includes a central microcomputer for data collection.

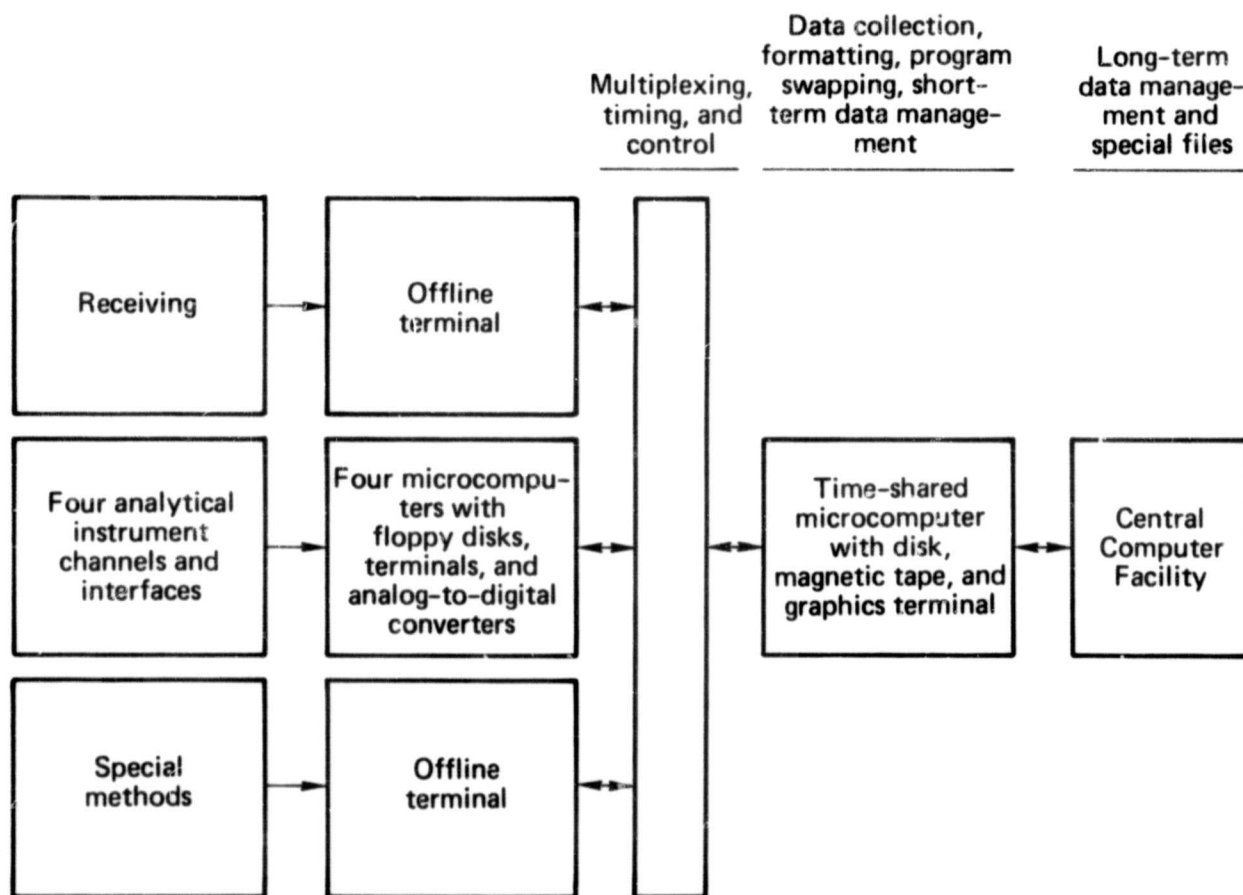


FIG. 3. System 2 point-to-point network, which incorporates a time-shared microcomputer with a mass-memory device.

The central microcomputer is equipped with disk, magnetic tape, and essential input/output devices. Additional input/output terminals are provided for the receiving section and other laboratory sections and for the entry of offline information and data into the data collection system.

A number of features should be incorporated into the system. The microcomputer should include a terminal with graphics capability, a mass-memory device (e.g., floppy disk) for each microcomputer, and a capability for programming in a high-level language. These features provide convenient operation and interaction, the capability to write and modify programs with relative ease, and facilities for backup storage of data.

The input/output terminals for offline use by the receiving section and non-automated instruments and methods should include local memory (floppy disks) for backup storage and, if equipped with cathode-ray tube (CRT) display, the ability to view selected lines of a large data set.

The data collection system should contain programs for the reduction of data entered from the offline instruments and special methods.

Variations of System 2

One variation of System 2 would be to provide two online microcomputer systems for the high-use analytical instruments and two "roll around" systems to be used where needed for current requested analyses. Such a system could be adopted instead of a hardwired microcomputer as shown in Fig. 3. The costs would be comparable to System 2.

Another variation of System 2 incorporates distributed microcomputers (Fig. 4). Each laboratory instrument has its own microcomputer for data acquisition, processing, and control. This allows any one of the microcomputers to be used for any instrument or special function when not busy otherwise. At this writing, automatic switching of the interconnected microcomputers from one duty to another is not fully proven, and the costs associated with this system are also comparable to those for System 2. With the rapidly advancing state of the art, automatic switching may well be available before the end of a several-year project and should be kept in mind.

A central microcomputer controls communications, the data base functions, and the expensive shared peripherals.

Advantages of System 2

The microcomputer system has the following advantages:

- The building-block units allow for orderly automation.
- Each unit provides data storage backup for each analytical instrument by means of a floppy disk.
- Each unit is relatively inexpensive. Thus, the laboratory is able to retain a standby unit in the event of failure of an online unit.
- The small dimensions and weight of each building-block unit permit roll-around automation systems that may be linked to an analytical instrument temporarily in high use.

Disadvantages of System 2

- A complete system for all instruments might be considered expensive.
- There is a limit to the memory in each microcomputer unit for storing a program. Certain instrumental methods require large applications programs that, if placed in a microcomputer system, would have to be segmented and chained into the core from a floppy disk, which may be too slow for good operation.
- Although a single microcomputer unit is relatively small when physically compared with a minicomputer, a number of them with peripherals may occupy too much space in the laboratory.
- A microcomputer system in the laboratory will be exposed to acid fumes, etc. Thus, each system may require an enclosure to protect it from the laboratory environment.
- The relatively large number of building blocks in the system increases the likelihood of maintenance problems.

System 3

System 3 (Fig. 5) is an expanded version of System 2. All instruments would have microcomputers for local data processing and control and be connected to a large central minicomputer. This complete system would include the four instruments mentioned for the other two alternatives and also the electron microprobe, the transmitting electron microscope, the ultraviolet-visible spectrophotometer, an electronic balance, a plate reader and data links for an inductively coupled plasma spectrometer, and a scanning electron microscope. In

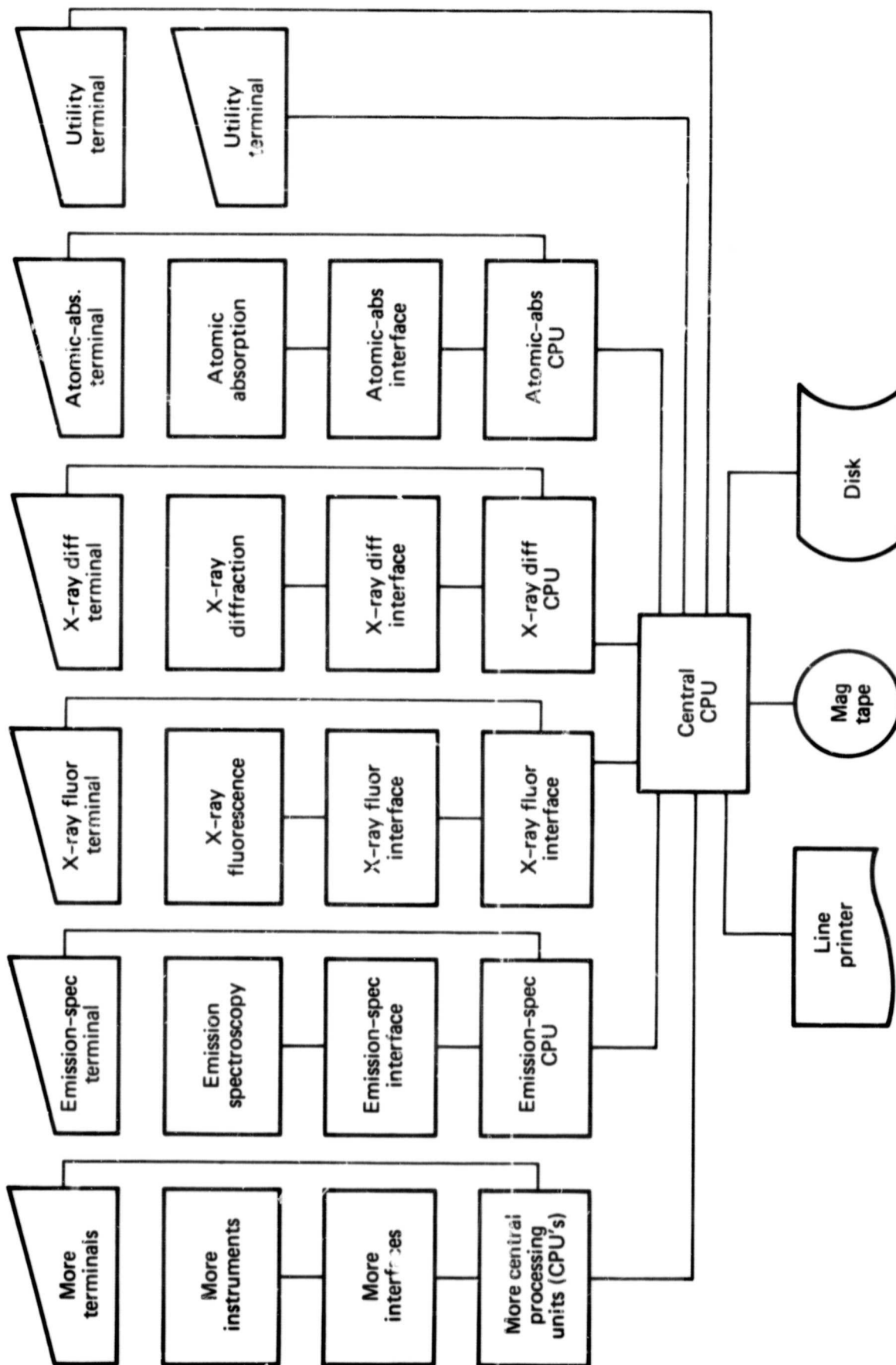


FIG. 4. System 2 interconnected network, which incorporates distributed microcomputers.

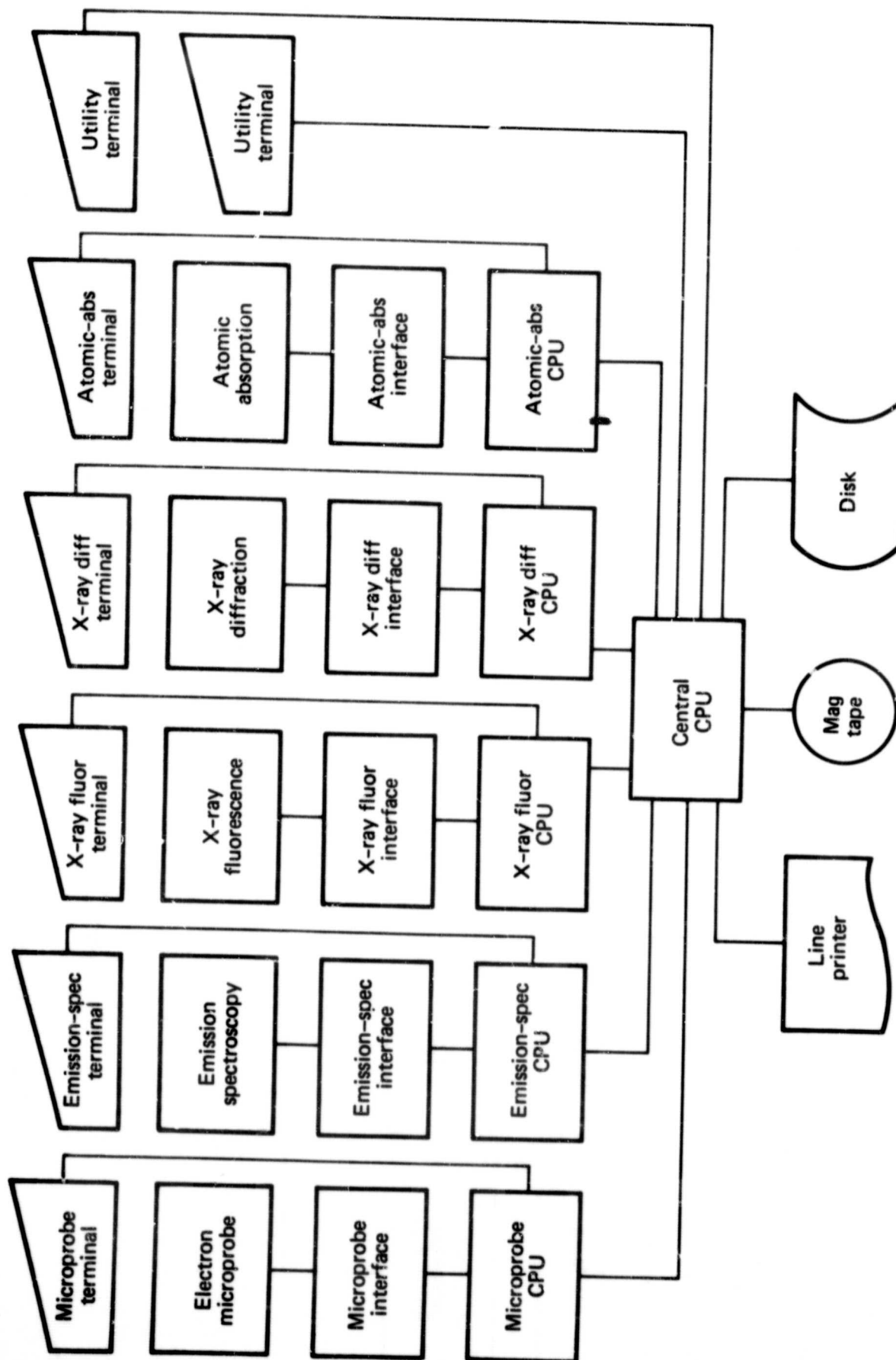


FIG. 5. System 3, the recommended ALS system, which is an expanded version of System 2. All instruments, which have microcomputers for local data processing and control, are connected to a large central minicomputer.

addition, complete software including data management software would be made available.

This system shows a later step in evolution under an orderly automation procedure.

In devising concepts of systems to fulfill ALS's requirements, the following three factors weigh heavily:

- The nature of the laboratory samples is such that the systems proposed must be capable of easily managing a variety of methods and programs for each instrument.
- Quality assurance requires reasonably capable computational ability and access to the historical record online.
- The capability to build the system in an orderly manner, gradually bringing new instruments into the system, is most important for this type of laboratory.

In view of the above factors, small multicomputer automation systems appear to be superior to a larger centralized computer automation system. They allow for automation of the most critical and most frequently run analyses as a first step, with the option to expand the system to a network of computers that includes other analyses and more complicated data management procedures.

The benefits of the alternative systems are discussed in the next section. Details of the costs and manpower effort saved are presented in the appendices. Although we show specific vendor equipment costs, these are not intended to reflect vendor recommendations, but rather to show typical costs for the items. The particular vendors should not be selected until definition of functional requirements for each component and implementation designs for the system are completed.

5. BENEFIT ANALYSIS

INTRODUCTION

Two alternate automation systems with variations have been proposed to fulfill ALS needs. In this section we summarize the benefits and expenses from the more detailed accounting found in appendices A, B, and C. Also, we include the cost of a completely automated system (Alternative 3).

BASIS FOR ANALYSIS

The number of determinations for each instrument is based on information furnished by ALS personnel for 1977. For some techniques we used estimates of the number of determinations based on a fraction of the original estimate since the proposed alternatives would not cover all methods on some of the instruments. This was especially true of x-ray diffraction, where there are a number of different procedures used, and emission spectroscopy, where there are two methods used. Also, the direct-reading emission spectrometer is online already, and some benefits from automation are now present.

Although quality control is not formalized because of the variety of samples analyzed by ALS, we have assumed that between 5 and 10% of the total analysis effort is devoted to quality control.

This study uses two alternate methods of computerization with variations. Both methods provide an ALS host central computing facility that would eventually take care of all the instruments surveyed. Both methods provide orderly automation, which could be extended as time and resources permit. The large initial cost of the centralized computer alternative must be viewed with the realization that it already contains much of the potential for future expansion. In part, the reason for the smaller apparent cost of the distributed microcomputer system is because in general one microcomputer will be used by each instrument, and all of the candidate instruments are not included in this study. A cost difficult to quantify, and not included in the centralized computer alternative, is the cost of disrupting existing operations each time a new instrument is added to the system. This hidden cost is not incurred with the distributed microcomputer system.

All of the alternatives contain some kind of data management facility either by direct processing or by communicating to the central computer facility of the Computer Services Division. We expect that daily logging of samples and the workload listing will be done locally and that statistical studies and special sorting will be done remotely.

We recommend that ALS automation be done by distributed microcomputers for the following reasons:

- The constantly changing mix of sample types demands a versatile, easily manipulated automation system.
- The large number of techniques used at one time or another suggest a system that can quickly be altered from one configuration to another.
- Since it is not reasonable to automate all the instruments at once, the microcomputer concept allows an orderly development of an eventually complete automation system.
- The provision of one added system as a backup replacement greatly enhances the availability of the system.
- The central computer concept is still preserved in the idea of a central microcomputer system for data recording and formatting and for program storage and exchange. A large central minicomputer could be used here as in Alternative 3, if the system some day grew too large for a central microcomputer.

Figure 5 presents the recommended ALS system, with the electron microprobe added to show how the system could be expanded into Alternative 3.

PROPOSALS

The recommended computer system initially automates four instruments and provides some data management capabilities. This might be considered phase 1 of the automation project, and as such, the costs are calculated on this basis.

We also suggest two joint development projects between LLL's chemistry departments and LeRC's ALS. One would be the development of a photographic plate reader, and the other would be the development of suitable search software for intensity (I) vs angle (2θ) x-ray diffraction data.

LLL's Ceramics and Metallurgy Division has expressed interest in such an effort. The cost and timetable of these projects would be developed as a part of the functional description phase of the individual proposals; however, the first phase of the automation project should be carried out with these proposals in mind.

BENEFITS

Table 1 summarizes benefits expressed as increased efficiency. We assumed a total effort of 0.3 full-time employee (FTE) for various quality control tasks, such as monitoring standards and running checks. We estimate that this effort is reduced by one-half with automation. The details of the rest of the benefits are in Appendix C.

A summary of one-time expenses is in Table 2, along with the expenses for Alternative 3, for an interim and a complete system. As mentioned above, the large initial price for the central computer system allows for future expansion.

Table 3 summarizes benefits vs expenses. We believe this is a conservative estimate. It only allows for those measurements and operations estimated from the previous year and for the four candidate instruments. Note that there are some benefits of computer automation that cannot be included in a

TABLE 1. Summary of estimated savings in work-time requirements at ALS with the proposed system.

	Full-time employee (FTE)
Atomic absorption	0.24
Emission spectroscopy	0.56
X-ray fluorescence	0.41
X-ray diffraction	0.40
Subtotal	1.61
Work-time saved by automated management functions	0.39
Subtotal	2.00
Work-time saved by quality control monitoring	0.15
Total	2.15

TABLE 2. Summary of one-time costs for the three options (thousands of dollars).

	Option 1: central computer with full data management	Option 1A: central computer with limited data management	Option 2: microcomputers at each instrument and central microcomputer	Option 3 (phase 1): microcomputers at each instrument and central computer with partial data management^a	Option 3 (complete): microcomputers at each instrument and central computer with full data management
Hardware and peripherals	120.5	102.9	85.4	225	364
Instrument interfaces	19.8	19.8	19.8	30	80
Software	186.0	186.0	156.0	230	665
Site preparation	20.0	20.0	20.0	30	40
Installation	33.5	33.5	33.5	50	60
Spare parts	16.0	10.0	10.0	15	20
Total	389.8	372.2	324.7	550	1229

^aIncludes microprobe and ultraviolet-visible spectrophotometer instruments plus a PDP-11/70 as the central computer.

TABLE 3. Summary of costs and work-time benefits.

	Option 1	Option 1A	Option 2
One-time system costs (thousands of dollars)	389.8	372.2	324.7
Outside maintenance (thousands of dollars)	11.2	9.7	9.6
Gross annual savings (FTE)	2.15	2.15	2.15
Annual expenditures (FTE)	0.60	0.35	0.35
Net annual savings (FTE)	1.55	1.8	1.8

cost factor study. Such benefits include fewer transcription errors, staff access to an easily programmable problem-solving computer, shorter turn-around time between sample in and report out, and more attention devoted to analytical methodology. In addition, the computer can be an educational tool of great value to analytical chemistry personnel if they have easy access to it. The large number of currently available calculational and statistical programs lend themselves to analytical applications and provide the analyst with the means for further pursuing automation studies.

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APPENDIX A. BREAKDOWN OF ONE-TIME COSTS FOR SYSTEMS AND THEIR VARIATIONS

COMPUTERS AND PERIPHERALS

The costs for the computers and peripherals for the three proposed automation systems and their variations are in Tables A-1 and A-2. Bear in mind that specific vendor equipment is presented to show typical costs and is not a recommendation.

The computer for the first option is an ECLIPSE C/330 as used in the current EPA and USGS systems. It may be used in a background time-shared foreground mode running under a real-time disk operating system. This mode of operation supports extended BASIC time-share automation. The C/330 also supports software for database management, communications to other computers, and an advanced operation system. The 128 kilobytes of core is recommended if an extensive data management system is to be used with this system. For the variation on this first option the smaller ECLIPSE S/230 has many of the same features, but lacks full data management capability.

For system 2 we use the DEC LSI-11 as a representative microcomputer. This is a powerful microcomputer system that also supports a time-shared environment.

For system 3, the complete system, we have used the PDP 11/70 as a representative central minicomputer. This system includes all instruments, a plate reader, and complete software for x-ray procedures and data management. Combined expenses for this system are in Table A-3.

We propose the following peripheral equipment for Option 1.

Disk Storage

The disk system provides a rapid-access storage of programs and data. We recommend a moving-head disk because of its fast data transfer properties. The proposed version for the first alternative incorporates the Data General model 6060 moving-head disk with a storage capacity of 96 megabytes.

TABLE A-1. Cost of computer hardware and peripheral equipment for Option 1.

	Cost (thousands of dollars)
Computer Data General ECLIPSE C/330, 128-kilobytes core memory and memory map	35.7
Moving-head disk, 96 megabytes	21.9
Magnetic tape, 9-track	8.4
Line printer, 300 lines/min	10.6
Papertape reader	1.7
System cabinet, 3-bay	3.0
Eight-line programmable multiplexor	4.1
Communications interface to LeRC's Central Computer Facility	2.0
Analog-to-digital converter, 16-channel	6.2
Advanced Operating System software	4.9
Other system software	1.0
Four Texas Instruments terminals @ \$1500 each	6.0
One graphics terminal	12.0
Two screen-type terminals	3.0
Total for Option 1	120.5
For Option 1A substitute:	
Computer Data General ECLIPSE/230, 96-kilobytes core memory and memory map without AOS software	23.0
Total for Option 1A	102.9

TABLE A-2. Cost of computer hardware and peripherals for Option 2.

	Cost (thousands of dollars)	Quantity	Total (thousands of dollars)
LSI-11 with 28-kilobytes core and dual floppy disks	4.95	5	24.3
Moving-head disk, DEC R-11-AR, 10 megabytes	8.9	1	8.9
Magnetic tape, DEC TMP-11VA, 9-track, 800 bits/in.	7.6	1	7.6
Line printer	15.0	1	15.0
System cabinet	0.37	4	1.5
Texas Instruments terminals	1.5	4	6.0
Screen terminal	1.5	2	3.0
Graphics terminal	12.0	1	12.0
Analog-to-digital converters, 14-bit	0.25	4	1.0
Subtotal			79.8
Software, RT-11, QJ013-AY			2.8
Software, BASIC, Q5913-AY			0.8
Software, FORTRAN, Q5980-AY			0.9
Software, Multitask, QJ945-AY			1.1
Subtotal			5.6
Total			85.4

Magnetic Tape

Magnetic tape is used as the primary backup medium for the system. It is also important for long-term bulk storage and for the transfer of data from one location to another.

Line Printer

The line printer is needed to produce workload listings, sample loading patterns, notebook results, final results and progress reports, as well as a listing of programs. The line printer should print at 300 lines/min.

Papertape Reader

The papertape reader is used for system startup and to load diagnostic programs when the disk or tape is not available.

Analog-to-Digital Converter System

The analog-to-digital converter reads signals coming from the automated instruments. The proposed converter has a resolution of one part in 16,384 (2^{14}) of a full-scale signal. We feel 16 channels should be present for system expansion and alternate use in case of malfunction.

Option 2 has similar peripheral equipment at the central microcomputer. Because each microcomputer has a dual-floppy disk system, a smaller central disk is specified. Also, a papertape reader is not specified here for the same reason. The analog-to-digital converter is a smaller version of the system proposed for Option 1. Since for Option 1 an analog-to-digital converter for each instrument is necessary, four will be required.

Both options require the same terminals.

Terminals

The terminals are the major means of entering information into the computer system other than the analog-to-digital converter. They are also used to report interim data and to issue warnings during automated runs.

We propose three different terminal types. One is a quiet hardcopy device. This is often used with the computer console to control system operation. A switch can be provided for background/foreground operation.

The second type of terminal is a CRT screen device. This type has the advantages of more rapid

TABLE A-3. Combined costs for System 3 (thousands of 1978 dollars).**NOTES:** PDP 11/70 includes full software licenses and a data management operating system.**PDP 11/03** includes twin floppy disks, cabinet, terminal, and analog-to-digital converter.**YEAR.#** indicates subcategories of expenses.

.0 Commercial hardware and software

.1 Specialized hardware

.2 Software development and documentation

.3 Site preparation such as air conditioning, electrical supply, etc.

.4 Installation

.5 Spare parts

Year.#	Item	Cost	Quantity	Total cost
1979.0	PDP 11/70	115	1	115
1979.0	Mag tape	15	1	15
1979.0	Lineprinter	15	1	15
1979.0	Disk storage	25	1	25
1979.0	DBMS system	10	1	10
1979.0	PDP 11/03	9	5	45
	Subtotal		10	225
1979.1	Atomic-absorption spectrophotometer (AAS) interface	5	1	5
1979.1	Emission spectroscopy (EMSPEC) interface	5	1	5
1979.1	Diano X-ray fluorescence (XRF) interface	5	1	5
1979.1	X-ray diffraction (XRD) interface	5	1	5
1979.1	Microprobe interface	5	1	5
1979.1	Ultraviolet-visible (UV-VIS) interface	5	1	5
	Subtotal		6	30
1979.2	DBMS software	50	1	50
1979.2	AAS software	25	1	25
1979.2	EMSPEC software	25	1	25
1979.2	Diano XRF software	25	1	25
1979.2	XRD software	40	1	40
1979.2	Microprobe software	10	1	10
1979.2	UV-VIS software	25	1	25
	Subtotal		7	200
1979.3	Site preparation	30	1	30
	Subtotal		1	30
1979.4	Installation	50	1	50
	Subtotal		1	50
1979.5	Spare parts	15	1	15
	Subtotal		1	15
	Year total		26	550
1980.0	PDP 11/03	9	5	45
1980.0	Lineprinter	15	1	15
1980.0	Graphics terminals	12	2	24
1980.0	XRD search system	25	1	25
	Subtotal		9	109
1980.1	Balance interface	5	1	5
1980.1	Inductively coupled plasma (ICP) interface	5	1	5
1980.1	Microprobe upgrade	25	1	25
	Subtotal		3	35
1980.2	Diano XRF software	25	1	25
1980.2	XRD software	40	1	40
1980.2	Balance software	25	1	25
1980.2	XRD search software	50	1	50

TABLE A-3. Continued.

Year.#	Item	Cost	Quantity	Total cost
1980.2	ICP software	10	1	10
1980.2	DBMS software	40	1	40
	Subtotal		6	190
1980.3	Site preparation	10	1	10
	Subtotal		1	10
1980.4	Installation	10	1	10
	Subtotal		1	10
1980.5	Spare parts	5	1	5
	Subtotal		1	5
	Year total		21	359
1981.0	Plate-reader system	30	1	30
	Subtotal		1	30
1981.1	Plate-reader interface	10	1	10
1981.1	Scanning electron microscope/transmission electron microscope (SEM/TEM) interface	5	1	5
	Subtotal		2	15
1981.2	Plate-reader software	150	1	150
1981.2	XRD search software	50	1	50
1981.2	SEM/TEM software	50	1	50
1981.2	Graphics software	25	1	25
	Subtotal		4	275
	Year total		7	320
	Grand total		45	1229

display and not creating large amounts of unneeded paper. Some have the ability to roll back, that is, redisplay information already scrolled off the screen.

A graphics terminal would also be provided for special uses. It should be an intelligent terminal similar to the Tektronix 4051.

We recommend seven terminals for the first two options: one graphic terminal and one CRT type for sample logging, four terminals (two of each type) for instruments and an extra terminal for the console.

INSTRUMENT INTERFACES

For Option 1 some of the existing interface designs from previous installations are applicable. For Option 2, however, it will be necessary to redesign the general computer interface. We anticipate that the existing laboratory instrument interface designs, where they exist, will be applicable to

either the LSI-11 system or the ECLIPSE system. Costs are summarized in Table A-4.

SOFTWARE

Option 1 assumes the application programs are written in Data General extended BASIC for a real-time disk operating system (RDOS) environment.

TABLE A-4. Summary of interface design and fabrication costs (thousands of dollars).

Type of interface	Option 1	Option 2
General interface design	—	6.0
General interface fabrication	9.3	9.3
X-ray fluorescence fabrication	3.0	3.0
X-ray diffraction fabrication	3.0	3.0
Atomic-absorption fabrication	1.5	1.5
Emission spectrometer fabrication	3.0	3.0

Option 2 assumes the application programs are written in LSI-11 BASIC or FORTRAN. For these latter options, FORTRAN or some other high-level language becomes a viable alternative because each instrument will be operating independently of the others. In any case, the language chosen for Option 2 will take advantage of software availability. At present, we expect x-ray application programs to be written in FORTRAN.

In the case of Option 1, existing laboratory application programs are available for the atomic-absorption instrument. We have estimated costs at about 20% of the original software cost for modifications that might be necessary. Programs also exist for emission spectroscopy. Modifications would be expected here also, and we estimate this cost to be comparable to atomic-absorption modifications. For Option 2, we estimate that translating the existing programs will double the cost.

The x-ray fluorescence programs have not been written for this system. We assume, however, some savings coming from modification of existing software that will be available from LLL's automation effort in metallurgy and ceramics, particularly for the matrix-correcting programs. Once the data is collected and corrected for matrix effects, the program for calculating answers follows a straightforward standards calibration curve. We estimate that these programs would contain about 1000 lines of BASIC or about one man-year of effort, or \$60,000. Adding 20% for modifying the existing matrix corrections programs brings the total to \$72,000. Much of this work will be available from

LLL, although it will probably have to be modified for Option 2. We estimate about half the above total will cover the high-level language for x-ray fluorescence for Option 1. For Options 2 and 3, the programs should be more readily available from LLL, and an estimate of half the cost of Option 1 seems reasonable.

The x-ray diffraction programs also have to be completely written. A situation similar to x-ray fluorescence can be anticipated. The complete x-ray diffraction program would have to be developed in steps, and the cost here is only for the first step (preparing a table of intensity vs 2θ values). Estimation comes from assuming twice the cost of the assembly language routines for x-ray fluorescence and about 40% more for the advanced language routines.

A good portion of the data management programs will come from those already established for the USGS automation project. We have estimated \$20,000 for this conversion for Option 1. In the case where data management will be done at the central computer facility, we assume that some of the cost will be borne by the computer facility and estimate \$20,000 here also. In any case, software protocol will have to be developed for communicating with this facility. We have estimated a total of \$10,000 for this software. Software is available for communicating with a central mini- or micro-computer and for networking. We estimate \$10,000 for implementing these systems. Table A-5 shows the estimated software costs for the different options.

TABLE A-5. Cost of computer software (thousands of dollars).

Description	Option 1		Option 2	
	Assembly	High-level	Assembly	High-level
Instrumentation Laboratory AA spectrophotometer	2.5	10	5	20
Jarrell-Ash 1.5-m emission spectrometer	2.5	10	5	20
Diano XRD-8000 x-ray fluorescence	15	36	8	18
X-ray diffraction (direct)	30	50	15	25
Data management		20		20
Link or network or both			10	
Communication to Central Computer Facility		10		10
Totals	50	136	43	113
Options 1 and 1A	186			
Option 2	156			

MISCELLANEOUS EXPENSES

These expenses include costs for site preparation, installation, spare parts, and test equipment. Expenses will vary somewhat for the option selected, but in general we estimate that these differences will not be appreciable except for software maintenance.

Site Preparation

For Option 1 this is the cost of preparing a room of about 200 ft² to house the computer, with adequate electrical service and air conditioning. It also includes pulling cables from instrument sites to the computer room. A nominal figure is \$20,000.

For Option 2, using microcomputers, the preparations would be somewhat different. But we will assume that \$20,000 covers such concerns as protecting the microcomputers from laboratory environment and establishing work areas.

Installation

This cost is estimated to be \$32,500, based on previous installations. It includes shipment of the system, installation at the ALS laboratory, hardware and software checkout, operational testing, and training personnel.

Spare Parts and Test Equipment

To maintain the system, a minimum complement of spare parts and test equipment must be acquired. Spare parts should include items such as control logic cards, power supplies, operational amplifiers, relays, and connectors. The cost for a recommended quantity of these items is about \$3,000. The major test equipment item, an oscilloscope, will cost about \$7,000. Thus, \$10,000 to \$20,000 should be set aside for spare parts and test equipment.

APPENDIX B. ADDED OPERATING COSTS FROM AUTOMATION

The proposed automation systems will add new costs to the annual operating costs of the ALS laboratory. These costs will mainly be for the maintenance of computer hardware and peripherals and for laboratory instrument hardware interfaces and software. The annual operating costs that reflect the above requirements for Options 1 and 2 are in Table B-1.

Software maintenance will depend on the option selected. For a full-fledged data management and operating system, we estimate 0.5 FTE. For maintenance of instrument software with data management at a remote facility, 0.25 FTE seems reasonable. Electronic maintenance of interfaces, cabling, and miscellaneous components will require another 0.1 FTE.

TABLE B-1. Annual operating costs and work-time for Options 1 and 2.

Category	Option 1A	Option 1B	Option 2
Vendor-supplied maintenance of computer, peripherals, and software (thousands of dollars)	11.2 ^a	9.7 ^a	9.6 ^b
In-house maintenance of interface hardware (FTE)	0.1	0.1	0.1
Same for software (FTE)	0.5	0.25	0.25
Total FTE	0.6	0.35	0.35

^aEstimated at 12% per year of computer hardware and peripherals not including terminals or software.

^bEstimated by Digital Equipment Corporation representative.

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APPENDIX C. DETAILED ASSESSMENT OF AUTOMATION BENEFITS

To assess the benefits that will accrue to ALS as a result of automation, we compared the manual effort (no automation) that will be required to meet the expected workload in the candidate instrumental analysis and sample coordination and management areas with the effort we project will be required if automation is implemented. Effort here is defined as the time required for an employee to perform a task and is expressed as multiple or fractional full-time employee (FTE) or both. We examined the detailed procedure tasks associated with the instrumental methods and sample management processes that are candidates for automation. For each candidate instrument, only those tasks that can be fully or partially automated will be more effort-efficient.

INSTRUMENTAL METHODS

We have adopted a model to calculate the effective time required of a chemist to make a determination using any of the candidate instruments. The model takes into consideration the multiple tasks that he must perform, including factors for quality control samples, reruns, and samples that are diluted. With the effective time, and the number of determinations per year, one can calculate the total chemist time in FTE to handle the workload.

The model is used to calculate the effort required for a single determination using manual techniques vs automated techniques. The effective total effort is then calculated, based on a linear relationship between the number of determinations and the effort per determination. It is possible, however, that this relationship would not extrapolate linearly to a higher number of determinations.

It should be remembered that it is the number of determinations that is used for these calculations, not the number of samples. Many samples require multiple analyses for the determination of each requested component, and some samples require several determinations to estimate one component.

The following two equations are used in the model:

$$t_s = p + (1 + f)(w + i + c) + fd, \quad (1)$$

where

t_s = total chemist time needed for each determination,

p = time for preparation of sample and log-book per determination,

w = time needed to write log and introduce sample per determination,

i = chemist time spent in operating the instrument per determination,

c = time needed to calculate and transcribe results per determination,

d = time taken for a single dilution,

and

f = fraction of off-scale samples requiring dilution;

and

$$e = t_s(1 + q)(1 + r) \frac{H}{H - T_b},$$

where

e = the effective chemist time taken per determination,

q = quality assurance fraction,

r = fraction of samples retested for reasons other than being off-scale,

H = total average operator time spent for a work session,

and

T_b = time to set up instrument at the beginning of each work session, shut it down at the end, and run standards.

With the model, calculations of the benefits to be realized by automation of the candidate instrumental methods appear in the following four subsections.

The Tables C-1 through C-5 give a breakdown of the tasks involved for each of the four instruments to be automated and a comparison of the effort that will be required by manual methods relative to the effort if automated techniques are developed.

TABLE C-1. Automation benefits: atomic-absorption spectrophotometer.

Task times and time factors	Symbol	At present	With automation
Preparation of sample (min)	p	4.9	4.9
Write log, introduce sample (min)	w	1.6	0.8
Operation of instrument by chemist (min)	i	2.0	2.0
Calculation & transcription of results (min)	c	4.9	0
Dilution of one off-scale sample (min)	d	5.0	4.0
Factor for samples diluted	f	0.2	0.2
Calculated chemist time per determination (min)	t _s	16.1	9.06
Retest factor	r	0.1	0.1
Quality control factor	q	0.1	0.1
Setup and shutdown per work session (min)	s	45	45
Hours per work session	H	6.5	6.5
Calculated effective chemist time per determination (min)	e	22.02	12.39
Benefit calculations			
Number of determinations per chemist day		21.8	38.73
Determinations per year		2734	2734
Chemist days per year to meet load		125	71
Chemist years to meet load (FTE)		0.56	0.31
(Effort efficiency improvement = 0.56 - 0.31 = 0.24 FTE)			

ATOMIC ABSORPTION SPECTROPHOTOMETER

We used the number of determinations for 1977 as a base for these figures.

EMISSION SPECTROSCOPY

We used 500 determinations/year as a figure for direct-reading emission spectroscopy. These figures compare an instrument already partially automated.

TABLE C-2. Automation benefits: emission spectrometer.

Task times and time factors	Symbol	At present	With automation
Preparation of sample (min)	p	27.0	27.0
Write log, introduce sample (min)	w	13.5	13.5
Operation of instrument by chemist (min)	i	108.0	54.0
Calculation & transcription of results (min)	c	27.0	0
Dilution of one off-scale sample (min)	d	5.0	5.0
Factor for samples diluted	f	0.05	0.05
Calculated chemist time per determination (min)	t	183.17	98.12
Retest factor	r	0.01	0.01
Quality control factor	q	0.05	0.05
Setup and shutdown per work session (min)	s	90	90
Hours per work session	H	6	6
Calculated effective chemist time per determination (min)	e	259.01	138.75
Benefit calculations			
Number of determinations per chemist day		1.85	3.46
Determinations per year		500	500
Chemist days per year to meet load		270	145
Chemist years to meet load (FTE)		1.2	0.64
(Effort efficiency improvement = 1.2 - 0.64 = 0.56 FTE)			

TABLE C-3. Automation benefits: x-ray fluorescence spectroscopy.

Task times and time factors	Symbol	At present	With automation
Preparation of sample (min)	p	9.31	9.31
Write log, introduce sample (min)	w	3.57	1.79
Operation of instrument by chemist (min)	i	5.0	3.0
Calculation & transcription of results (min)	c	4.89	0
Dilution of one off-scale sample (min)	d	5.0	5.0
Factor for samples diluted	f	0.17	0.17
Calculated chemist time per determination (min)	t	25.91	15.76
Retest factor	r	0.1	0
Quality control factor	q	0.1	0.1
Setup and shutdown per work session (min)	s	95	95
Hours per work session	H	4.0	4.0
Calculated effective chemist time per determination (min)	e	51.89	28.7
Benefit calculations			
Number of determinations per chemist day		9.25	16.72
Determinations per year		1891	1891
Chemist days per year to meet load		204	113
Chemist years to meet load (FTE)		0.91	0.5
(Effort efficiency improvement = $0.91 - 0.5 = 0.41$ FTE)			

X-RAY FLUORESCENCE SPECTROSCOPY

We used the figure for the number of determinations for 1977.

X-RAY DIFFRACTION BY DIRECT READING

For this study we estimate about 1000 determinations are run by this method, which seems to

TABLE C-4. Automation benefits: x-ray diffraction.

Task times and time factors	Symbol	At present	With automation
Preparation of sample (min)	p	9.0	9.0
Write log, introduce sample (min)	w	1.2	1.2
Operation of instrument by chemist (min)	i	4.8	2.0
Calculation & transcription of results (min)	c	36.0	6.0
Dilution of one off-scale sample (min)	d	0	0
Factor for samples diluted	f	0	0
Calculated chemist time per determination (min)	t	51.0	18.2
Retest factor	r	0.01	0.01
Quality control factor	q	0.1	0.1
Setup and shutdown per work session (min)	s	36.0	36.0
Hours per work session	H	4.0	4.0
Calculated effective chemist time per determination (min)	e	66.66	23.79
Benefit calculations			
Number of determinations per chemist day		7.2	20.18
Determinations per year		1000	1000
Chemist days per year to meet load		139	50
Chemist years to meet load (FTE)		0.62	0.22
(Effort efficiency improvement = $0.62 - 0.22 = 0.4$ FTE)			

TABLE C-5. Management Tasks.

Tasks	Present effort (FTE)	Effort with automation (FTE)
Gathering information for the coordination of laboratory activities	0.38	0.19
Preparing reports of laboratory activities	0.25	0.12
Monitoring quality control	0.13	0.06
Total	0.76	0.37
(Effort efficiency improvement = 0.39 FTE)		

correspond to the statistical data furnished. This is for partial automation. The final matching of intensity vs 20 values would be computer-assisted but not completely automatic.

The estimates in Table C-5 are for an interactive management system that would allow a reduction of about half the current effort in monitoring laboratory functions.